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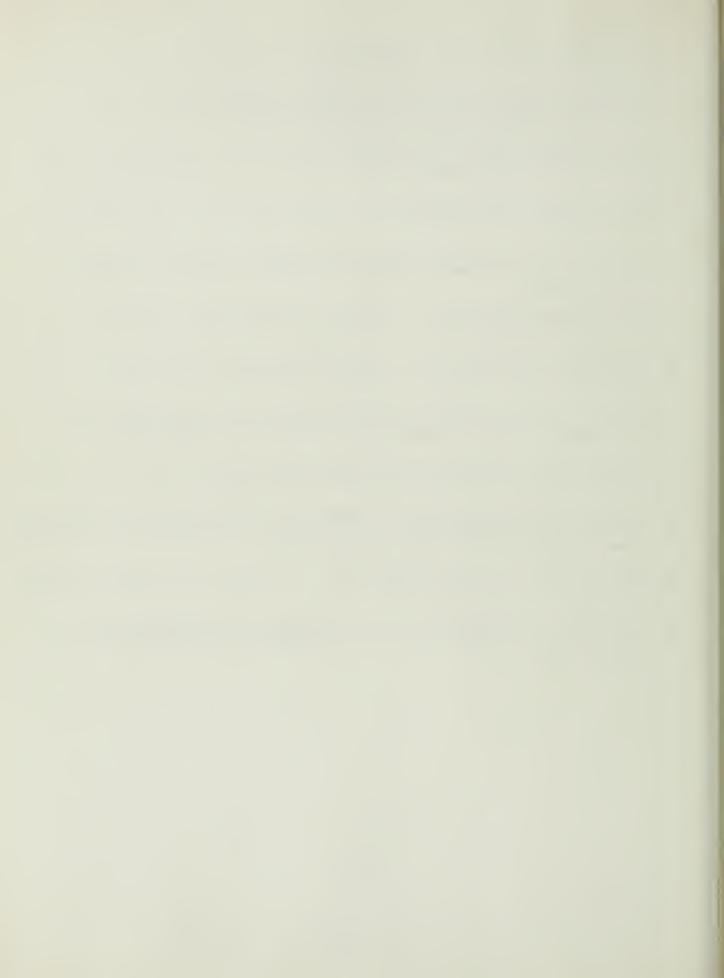
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NUMERICAL QUADRATURE OVER A RECTANGULAR DOMAIN IN TWO OR MORE DIMENSIONS

by

J. C. P. Miller

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Numerical Quadrature over a Rectangular Domain

in Two or More Dimensions

By J.C.P. Miller

III Quadrature of a Harmonic Integrand

Introductory

1. In Note I(1), §5, formula (B), §7, formula (B'), and in §9, also in Note II(1) in several places, we have seen how the error term is very much reduced if the integrand f(x,y) is a harmonic function, that is, if $\nabla^2 f = 0$. In this note we pursue further this special case, in which especially high accuracy is attainable with few points.

It may not be often that the integrand will have this special form, but it seems worthwhile to develop a few of the interesting formulae. We start by obtaining expansions for n variables, and more extensive ones for two variables, and then obtain and consider special quadrature formulae.

2. Expansions. As in II(1), § 2, we develop $f(x_1, x_2, ..., x_n)$ as a Taylor series in even powers of each of the variables x_r . Then, using $\nabla^2 f_0 = 0$ whenever it is applicable, we obtain

where, as before, extended,

$$(2.2) \mathcal{D}^{4} f_{0} = \sum \frac{\partial^{4} f_{0}}{\partial x_{r}^{2} \partial x_{s}^{2}} \qquad \mathcal{D}^{6} f_{0} = \sum \frac{\partial^{6} f_{0}}{\partial x_{r}^{2} \partial x_{s}^{2} \partial x_{t}^{2}} \qquad \mathcal{D}^{8} f_{0} = \sum \frac{\partial^{8} f_{0}}{\partial x_{r}^{2} \partial x_{s}^{2} \partial x_{t}^{2} \partial x_{u}^{2}}$$

etc., the summations extending over all possible combinations of r, s, t,...with no two equal.

(1) J.C.P.Miller, M.T.A.C., in the press.



We have likewise, labelling the symmetrical sets of points as in Note II, the expansions for sums of values of f over the sets

$$(2.31) \ 0 \ f_0$$

$$(2.32) \ \alpha(a) \ 2nf_0 - \frac{h_1h_1^{h_1}a_1^{h_1}}{h_1!} \mathcal{F}^h f_0 + \frac{6n_0^6a_0^6}{6!} \mathcal{F}^6 f_0 + \frac{h_1h_0^8a_0^8}{8!} (\mathcal{F}^6 - 2\mathcal{F}^8) f_0$$

$$-\frac{10h_0^{10}a_1^{10}}{10!} (\mathcal{F}^h \mathcal{F}^6 - 2\mathcal{F}^{10}) f_0 - \frac{2h_1^{12}a_1^{12}}{12!} (2\mathcal{F}^{12} - 3\mathcal{F}^{12} - 6\mathcal{F}^{12}\mathcal{F}^8 + 2\mathcal{F}^{12}) f_0 + \dots$$

$$(2.33) \ \beta \ (b) \ 2n(n-1)f_0 - \frac{8h_1^{h_0}b_1^{h_1}}{h_1!} (n-h)\mathcal{F}^h f_0 + \frac{12h_0^6b_0^6}{6!} (n-16)\mathcal{F}^6 f_0$$

$$+\frac{8h_0^8b_0^8}{8!} \left\{ (n+6)\mathcal{F}^8 - 2(n-6h)\mathcal{F}^8 \right\} f_0 - \frac{20h_0^{10}b_0^{10}}{10!} \left\{ (n-h)\mathcal{F}^h \mathcal{F}^6 - (n-256)\mathcal{F}^{10} \right\} f_0$$

$$-\frac{h_1^{12}b_0^{12}}{12!} \left\{ 2(n-3h) \mathcal{F}^{12} - 3(n+362) \mathcal{F}^{12} - 6(n-728) \mathcal{F}^h \mathcal{F}^6 - (n-256)\mathcal{F}^{10} \right\} f_0$$

$$(2.34) \mathcal{F} (c,d) \ 4n(n-1)f_0 - \frac{8h_0^4}{4!} \left\{ (n-1)(c^h + d^h) - 6c^2d^2 \right\} \mathcal{F}^h f_0 + \frac{12h_0^6}{6!} \left\{ (n-1)(c^h + d^h) - 15c^2d^2(c^h + d^h) \right\} \mathcal{F}^6$$

$$+ \frac{8h_0^8}{8!} \left\{ (n-1)(c^8 + d^8) - 28c^2d^2(c^h + d^h) + 70c^h d^h \right\} \mathcal{F}^8$$

$$-2\left\{ (n-1)(c^8 + d^8) - 28c^2d^2(c^h + d^h) - 70c^h d^h \right\} \mathcal{F}^6$$

$$+ \dots$$

$$(2.35) \mathcal{E} (e) \ \frac{h}{3}n(n-1)(n-2)f_0 - \frac{8h_0^4 e^h}{4!} (n-2)(n-7) \mathcal{F}^h f_0 + \frac{12h_0^6 e^h}{6!} (n^2 - 33n + 122) \mathcal{F}^6 f_0$$

$$+ \frac{8h_0^8 e^8}{8!} \left\{ (n-2)(n+13) \mathcal{F}^8 - 2(n^2 - 129n + 109h) \mathcal{F}^8 \right\} f_0 + \dots$$

We recall that 0 is the origin, or centre of the square, α (a) includes all points with one coordinate \pm ah and the rest zero, $\beta(b)$ has two coordinates each independently \pm bh and the rest zero, $\delta(c,d)$ has one coordinate \pm ch, another \pm dh and the rest zero and finally $\mathcal{E}(e)$ has three coordinates each independently \pm eh with the rest zero.

3. Expansions over a square are simpler since \mathcal{F}_0 , \mathcal{Q}_0^8 etc. vanish. They can be obtained by analysis with the detached operators - in particular \mathcal{T} ; we proceed to obtain expansions with general terms.



If F(z) = u + iv is a function of a complex variable z = x + iy then both u and v are harmonic functions satisfying $D_x^2\phi + D_y^2\phi = 0$. Likewise, if u is a harmonic function, it can be shown that v exists such that u + iv is a function of a complex variable. We then have

$$D_y F = iF' = iD_n F$$

and

(3.1)
$$D_x D_y = \Re^2 = iD_x^2 = -iD_y^2$$

In order to develop expansions we therefore substitute

(3.2)
$$D_x = i^{-1/2} D_y = i^{1/2} D_y$$

Consider, firstly

(3.3)
$$J = (2h)^{-2} \int_{-h}^{h} \int_{-h}^{h} f(x,y) dx dy = \frac{1}{4h^2 D_x D_y} (e^{hD_x} - e^{-hD_x}) (e^{hD_y} - e^{-hD_y}) f_0$$

The operator is

$$(3.4) \begin{cases} \frac{\sinh h^{D_{X}} \sinh h^{D_{Y}}}{h^{2} D_{X} D_{Y}} &= \frac{\sinh i^{-1/2} h^{D_{X}} \sinh i^{1/2} h^{D_{X}}}{h^{2} D^{2}} \\ &= \frac{1}{2} \frac{\cosh (i^{1/2} + i^{-1/2}) h^{D_{X}} - \cosh (i^{1/2} - i^{-1/2}) h^{D_{X}}}{h^{2} D^{2}} \\ &= \frac{1}{2} \frac{\cosh \sqrt{2} h - \cos \sqrt{2} h^{D_{X}}}{h^{2} D^{2}} \end{cases}$$

whence

(3.5)
$$J = (\frac{2}{2!} + \frac{2^3h^4}{6!} \Re^4 + \frac{2^5h^8}{10!} \Re^8 + \dots + \frac{2^{2r+1}h^{4r}}{(4r+2)!} \Re^4 + \dots) f_0$$

Likewise
$$(x_{\alpha}, y_{\alpha}) = (e^{-ahD}_{x} + e^{-ahD}_{y} + e^{-ahD}_{y}) f_{0}$$

$$= 2 (\cosh ah D_{x} + \cosh ah D_{y}) f_{0}$$

$$= 2 (\cosh i^{-1/2} ahD + \cosh i^{1/2} ahD) f_{0}$$

$$= 4 \cosh \frac{ah}{\sqrt{2}} \cos \frac{ah}{\sqrt{2}} f_{0}$$

$$= 4 \left[1 - \frac{a^{4} h^{4}}{4^{3}} D^{4} + \frac{a^{8}h^{8}}{8!} D^{8} + ... + (-1)^{r} \frac{a^{4}rh^{4}r}{(4r)!} D^{4}r + ... \right] f_{0}$$



and
$$\sum_{\beta(b)} f(x_{\beta}, y_{\beta}) = 4 \cosh bh D_{x} \cosh bh D_{y} f_{0}$$

$$= 4 \cosh i^{-1/2}bh \cosh i^{1/2} bh f_{0}$$

$$= 2 (\cosh bh \sqrt{2} h + u bh \sqrt{2} h) f_{0}$$

$$= 4 \left[1 + \frac{2^{2} b^{1} h^{4}}{4!} h^{4} h + \frac{2^{4} b^{8} h^{8}}{8!} h^{8} + ... + \frac{2^{2r} b^{4r} h^{4r}}{(4r)!} h^{4r} + ...\right] f_{0}$$

We shall not use all the expansions given above in the present note, but it seems useful to set out the collected results for future use.

4. <u>Lattice-point formulae over a Square</u>. We consider first formulae in two variables, and start with 9 points, putting a = b = 1 and using the sets 0, $\alpha(1)$, $\beta(1)$. We write

(4.1)
$$J = I/4h^2 = A_0 f(0,0) + \sum A_{\alpha} f(x_{\alpha}, y_{\alpha}) + \sum A_{\beta} f(x_{\beta}, y_{\beta})$$
 using (x_{α}, y_{α}) etc. as typical sets of coordinates. Using (3.5) - (3.7), we equal coefficients of $\sum_{\alpha}^{h_{\alpha}} f(x_{\beta}, y_{\beta})$

This gives

with correction term $C = -(-4 A_{\alpha} + 256 A_{\beta} - \frac{64}{91}) \frac{h^{12}}{12!} \frac{12}{D} f_0$

We obtain the formula

(4.3)
$$7 - 32 7 \div 900$$

-32 1000 -32 with main correction term- $\frac{1952}{1365} \frac{h^{12}}{12!} \times 12 f_0$

This formula is remarkably good. With the example of Part I, we have, writing $J' = h^2 J$

$$J' = \frac{1}{4} \int_{0}^{1.2} \int_{0}^{1.2} \sin x \sinh y \, dx \, dy = \frac{1}{4} (1 - \cos 1.2)(\cosh 1.2 - 1)$$

$$= 0.12922 \ 70590 \ 73675 \ 11602$$

Formula (4.3) gives $J' \neq 0.12922 70590 72834 11029$ with $E = -0.0^{12}841 00573$ and $C = +0.0^{12}841 01633$.



5. Five-point formulae. The high precision of (4.3) suggests that formulae of lessor precision, with fewer points, may be useful. We use the first two of (4.2) and take one of A_0 , A_{α} , A_{β} to be zero (i) $A_0 = 0$ gives an eight-point formula with relatively poor precision.

(5.1)
$$19$$
 56 19 \div 300
56 0 56
19 56 19 with main correction term $-40 \frac{h^8}{9!} R^8$ f₀
(ii) $A_{\infty} = 0$ gives

(ii) $A_{\alpha} = 0$ gives

(iii) $A_{\beta} = 0$ gives

We observe that (5.2) and (5.3) combine in the proportions $\frac{7}{15}$: $\frac{8}{15}$ to give (4.3), though without an error estimate! Likewise $\frac{7}{3} \times (5.2) - \frac{4}{3} \times (5.3)$ gives (B) of Note I, and an estimate for the correction, namely $-\frac{112}{5}$ $\frac{h^8}{9!}$ \mathbb{R}^8 f_0 when (x,y) is harmonic.

Another combination, that of (5.2) and (5.3) in equal proportions gives a small correction term:

Again 4 X (5.2) - 3 X (5.3) gives small multipliers:

(5.5)
$$\begin{bmatrix} 1 & 3 & 1 & \div 15 \\ 3 & -1 & 3 \\ 1 & 3 & 1 \end{bmatrix}$$
 with main correction term $-\frac{212}{5} \frac{h^8}{9!} \Re^8 f_0$



Evidently (4.3) is most precise, but simultaneous use of (5.2) and (5.3) gives an idea of the precision attained and readily yield the better result if desired. Formula (5.5) might be helpful with desk computing but (5.1) has little to recommend it.

Numerical results for some of the formulae using the example of \S 4 are as follows:

Formula.	Result J'	10 ¹⁰ X-E.	10 ¹⁰ X C
(5.1)	0.12922 72986	+2395	-2396
(5.2)	0.12922 70974	+ 383	- 383
(5.3)	0.12922 70255	- 336	+ 335
I (B)	0.12922 71932	+1341	+1342
(5.4)	0.12922 70615	+ 24	- 24

6. General n; $2n^2 + 1$ points. We consider now the n-dimensional case, $n \geq 3$, using lattice points 0, $\alpha(1)$, $\beta(1)$. In this case the term in \mathcal{F}_0^6 is relevant, and the \mathfrak{L}_0^8 f term will appear in the error, except when n=3.

We equate coefficients of f_0 , $\mathcal{D}^4 f_0$, $\mathcal{D}^6 f_0$ in the expansions resulting from use of (2.1), (2.31)-(2.33) in (4.1). We obtain

(6.1)
$$\begin{cases} A_0 + 2n A_{\alpha} + 2n(n-1) A_{\beta} = 1 \\ -4 A_{\alpha} - 8(n-4) A_{\beta} = \frac{4}{15} \\ +6 A_{\alpha} + 12(n-16) A_{\beta} = \frac{16}{21} \end{cases}$$

while
$$C = -\{4 A_{\alpha} + 8(n+6)A_{\beta} - \frac{16}{45}\}\frac{h^8}{8!} \Re^8 f_0 + \{8A_{\alpha} + 16(n-64)A_{\beta} + \frac{192}{45}\}\frac{h^8}{8!} 2^8 f_0$$

These yield

(6.2)
$$A_0 = \frac{-6\ln^2 + 93\ln + 3780}{3780} \quad A_\alpha = \frac{6\ln -496}{3780} \quad A_\beta = \frac{-61}{7560}$$
with
$$C = \frac{1198}{945} \quad \frac{h^8}{8!} \approx 6 \quad f_0 + \frac{3619}{315} \quad \frac{h^8}{8!} 2^8 f_0$$

In particular

(6.33)
$$n = 3$$
 $A_0 = \frac{12048}{7546}$ $A_{\alpha} = -\frac{626}{7560}$ $A_{\beta} = -\frac{61}{7560}$
(6.34) $A_{\alpha} = -\frac{626}{7560}$ $A_{\beta} = -\frac{61}{7560}$

(6.34)
$$n = 4$$
 $A_0 = \frac{13056}{7560}$ $A_{\alpha} = -\frac{504}{7560}$ $A_{\beta} = -\frac{61}{7560}$



(6.35)
$$n = 5$$
 $A_0 = \frac{13820}{7560}$ $A_{\alpha} = -\frac{382}{7560}$ $A_{\beta} = -\frac{61}{7560}$

(6.36)
$$n = 6$$
 $A_0 = \frac{1 + 3 + 0}{7560}$ $A_{\alpha} = -\frac{260}{7560}$ $A_{\beta} = -\frac{61}{7560}$

As a numerical illustration for n = 3 we consider

$$J = \frac{1}{8} I = \frac{1}{8} \int_{-1}^{1} \int_{-1}^{1} \int_{-1}^{1} \cos \frac{3}{4} x \cos y \cosh \frac{5}{4} z dx dy dz$$

$$= \frac{16}{15} \sin \frac{3}{4} \sin 1 \sinh \frac{5}{4} = 0.9800827$$

Formula (6.33) gives J = 0.9799734 with E = -0.0000109 and C = +0.0000110. This result is less spectacular than that of §4, for these reasons:

- i) In $\S4$, h = 0.6, here h = 1, and the correction term in (4.3) contains a high power of h.
- ii) The correction term in (6.2) is of order h⁸, that in (4.3) is of order h¹²
- iii) The higher the number of dimensions, the more individual terms there are in $\mathcal{D}^8 f$, $\mathcal{D}^{12} f$, etc. In (4.3) there is only one term in $\mathcal{D}^{12} f$, in (6.33) there are 9 in $\mathcal{D}^8 f$.
- iv) The effect of larger interval h is enhanced by the use of the factor $\frac{5}{4}$, which exceeds unity, in $\cosh \frac{5}{4}$ Z; this is only partially balanced by the factor $\cos \frac{3}{4}$ x.

In spite of these points, the formula (6.2) seems a good one.

7. Quadrature over a square; specially chosen points. Since the expansions of §3 involve only cross-differences \mathfrak{D}^h f_0 , it appears likely that use of sets of diagonal points β will be more profitable than attempts to use sets α . It turns out that sets 0, $\alpha(a)$, $\beta(b)$ and 0, $\alpha(a)$ both fail to give real values of α if maximum precision is sought. On the other hand, we can get several formulae making use of any number of sets $\beta(b_p)$, p = 0(1) r, both with and without the point 0.

We start first with r sets β (b_p), without the point 0. We have to find the 2r constants A_{β_b} , b_p satisfying the equations

(7.1)
$$\sum_{p=1}^{r} 4A_{\beta_p} b_p^{4(s-1)} = \frac{1}{(2s-1)(4s-3)} = C_{s-1}, \quad s = 1(1) \ 2r$$

obtained by substitution of (3.5) - (3.7) in

(7.2)
$$J = \sum A_{\beta_{\flat}} f \left(\pm b_{\flat} h, \pm b_{\flat} h \right)$$



and equating the coefficients of the first 2r coefficients of \mathfrak{D}^4 . Sundry powers of 4 have been cancelled.

By familiar arguments, the bp are roots of the equation

(7.3)
$$\begin{vmatrix} 1 & x & x^2 & x^r \\ c_0 & c_1 & c_2 & c_r \\ c_1 & c_2 & c_3 & c_{r+1} \\ c_r & c_{r-1} & c_{r-2} & c_{2r-1} \end{vmatrix} = 0$$

These are the orthogonal polynomials corresponding to the weight function $w(x) = \frac{1}{2} (x^{-3/4} - x^{-1/2})$ for range $0 \le x \le 1$. The first two are

(7.4)
$$\begin{cases} 15x - 1 = 0 \\ 819x^2 - 438x + 11 = 0 \end{cases}$$

The main correction term is obtained from the next power of \mathfrak{D}^{4} and yields

(7.5)
$$C = (C_{2r} - \sum_{b=1}^{r} 4 A_{bb} b_{b}^{8r}) \frac{2^{4r} h^{8r} b^{8r}}{(8r)!}$$

If the point 0 is included, our equations (7.1) are replaced by

(7.6)
$$\begin{cases} A_0 + \frac{4\Sigma A}{4\Sigma A} = 1 \\ p = 1 \\ p = 1 \end{cases} = 1$$

$$p = 1 \quad A_{\beta p} \quad b_p^{4s} = \frac{1}{(2s+1)(4s+1)} = C_s, \quad s = 1(1) \ 2r$$

and the b_p^{μ} are roots of the equation

$$\begin{vmatrix} 1 & x & x^{2} & x^{r} \\ c_{1} & c_{2} & c_{3} & c_{r+1} \\ c_{2} & c_{3} & c_{4} & c_{r+2} \\ c_{r+1} & c_{r+2} & c_{r+3} & c_{2r} \end{vmatrix} = 0$$



which are the orthogonal polynomials for the weight function $w(x) = \frac{1}{2}(x^{1/4}-x^{1/2})$ for the range $0 \le x \le 1$. The first two are

$$3x - 1 = 0$$

$$17017x^{2} - 13650x + 1745 = 0$$

The main correction term is this time

(7.9)
$$C = (C_{2r+1} - \sum_{b=1}^{r} 4 A_{b} b_{b}^{8r+4}) \frac{2^{2r+1} b^{4r+2}}{(4r+2)!} \mathcal{D}^{4r+2}$$

In each case the coefficients A_{β_r} may be computed by standard methods.

8. Formulae for r = 1. These have 4 and 5 points respectively

(8.1)
$$A_{\beta} = \frac{1}{4}$$
 $b = 15^{-1/4}$ $C = \frac{64}{225}$ $\frac{h^8 \mathcal{D}^8}{8!} f_0$

(8.2)
$$A_0 = \frac{14}{5}$$
 $A_\beta = \frac{1}{20}$ $b = 3^{-1/4}$ $C = \frac{2816}{12285}$ $\frac{h^{12} \Re 12}{12!} f_0$

Written out in full:

(8.3)
$$J = \frac{1}{4} I = \frac{1}{4} \left\{ f(15^{-1/4}, 15^{-1/4}) + f(-15^{-1/4}, 15^{-1/4}) + f(15^{-1/4}, -15^{-1/4}) + f(-15^{-1/4}, -15^{-1/4}) \right\}$$

$$(8.4) \quad J = \frac{1}{4} I = \frac{4}{5} f(0,0) + \frac{1}{20} \left\{ f(3^{-1/4}, 3^{-1/4}) + f(-3^{-1/4}, 3^{-1/4}) + f(3^{-1/4}, -3^{-1/4}) + f(-3^{-1/4}, -3^{-1/4}) + f(-3^{-1/4}, -3^{-1/4}) + f(-3^{-1/4}, -3^{-1/4}) \right\}$$

As a numerical test use

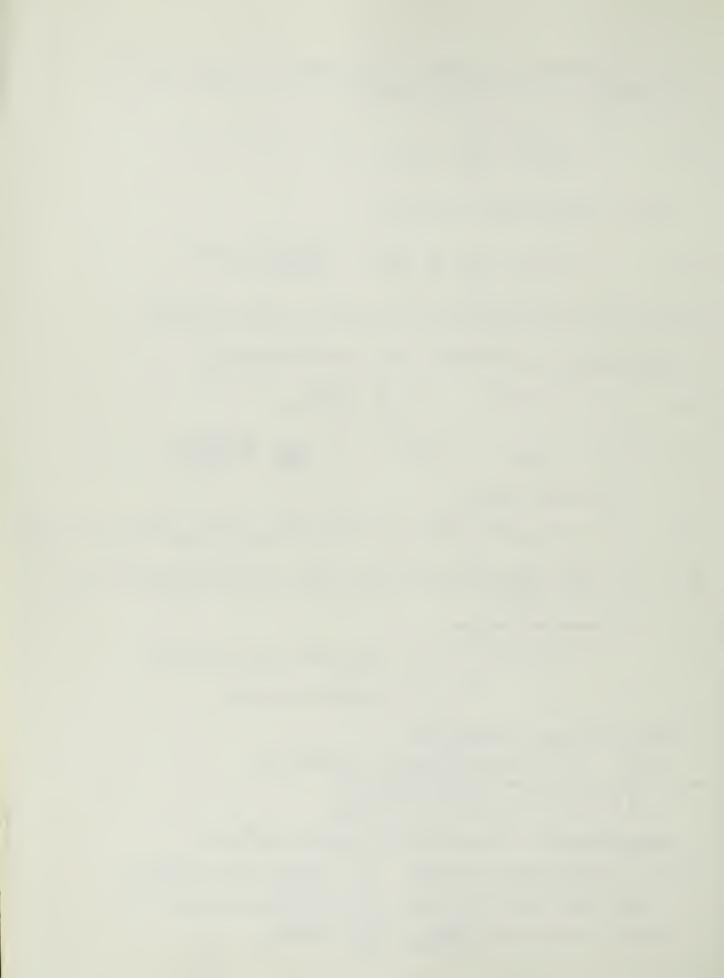
$$J = \frac{1}{4} I = \frac{1}{4} \int_{-1}^{1} \int_{-1}^{1} \cos x \cosh y \, dy = \sin 1 \sinh 1$$
$$= 0.98889 77057 62865$$

Formula (8.3) gives 0.98889 06525

with
$$E = 0.0000070533$$
 and $C = +0.0000070547$

and formula (8.4) gives 0.98889 77062 41358 with $E = +0.0^9478493$ and $C = -0.0^9478543$.

9. Formulae for r = 2. These have 8 and 9 points respectively



formula (9.1) gives 0.98889 77057 62853 38396

with $E = -0.0^{13}$ 1171243 and $C = +0.0^{13}$ 1171555 while formula (9.2) gives 0.98889 77057 62865 09647 with $E = +0.0^{19}$ 9 and $C = 0.0^{19}$ 90

With formula (9.2) we find approximately 0.82447 37090 77903 16756 for

$$\frac{1}{16} \int_{-2}^{2} \int_{-2}^{2} \cos x \cosh y \, dx \, dy = \sin 2 \sinh 2$$

$$= 0.82447 37090 77809 15433$$

with $E = 0.0^{13}9401323$ and $C = 0.0^{13}9406250$.

These formulae clearly have high precision, even with considerable values of h.

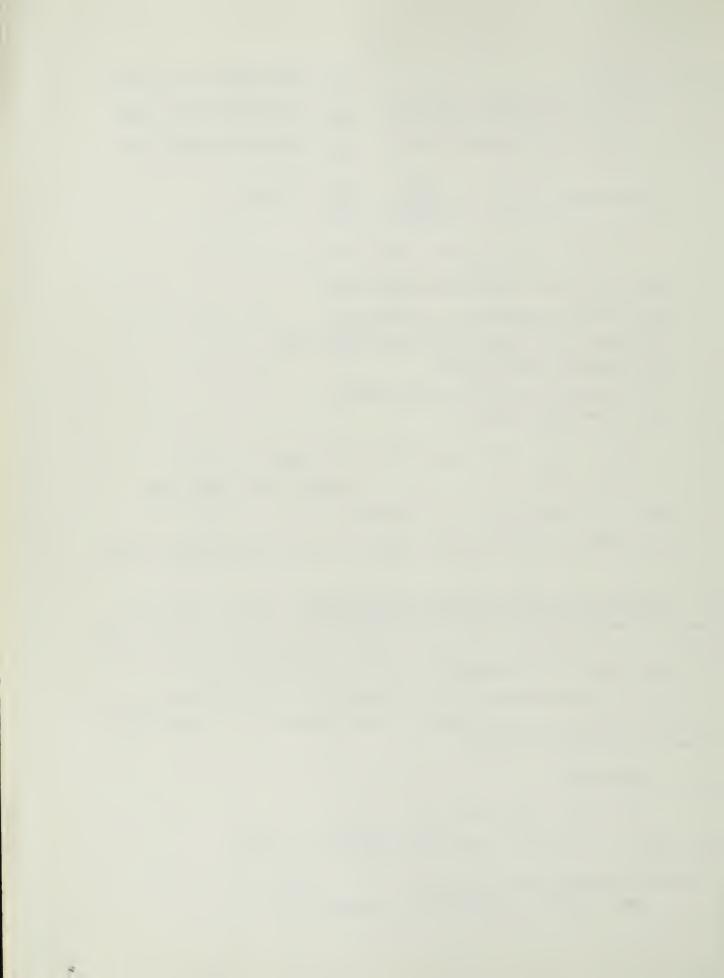
10. Quadrature over a Cube; specially chosen points. The search for such formulae is more difficult in 3 or more dimensions. It seems that one or more extra available constants are needed in order to obtain real points. We shall not pursue this, but give one simple formula for three dimensions.

We find nothing convenient by use of points $\alpha(a)$, with or without 0; likewise 0 with $\beta(b)$ fails to give real points. We can, however, use 12 points $\beta(b)$ alone. We have then to satisfy

(10.1)
$$\begin{cases} 2n(n-1)A_{\beta} = 1 \\ 8b^{4}(4-n)A_{\beta} = \frac{4}{15}, \text{ where } n = 3. \end{cases}$$

This yields $b = (2/5)^{1/4} = 0.79527 07287 67051 A_B = 1/12$

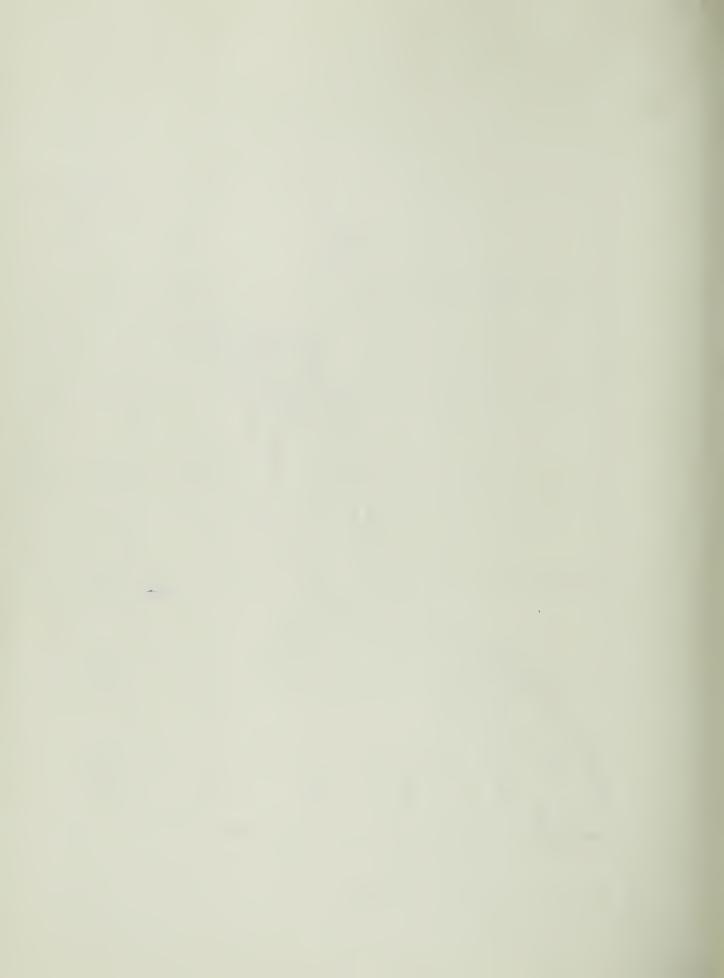
with main correction term $C = (156 \text{ b}^6 \text{ A}_{\beta} + \frac{16}{21}) \frac{\text{h}^6}{6!} \mathcal{I}^6 \text{ f}_0 = 0.00562 \text{ h}^6 \mathcal{I}^6 \text{ f}_0$



With the example of $\S6$, with integrand $\cos \frac{3}{4} \times \cos y \cosh z$ (10.1) gives J = 0.97519 with E = -0.00489 and C = +0.00494.

The only formula found that allows for the term J^6 f_0 and has an error of order h^8 is (6.33), which needs 9 points. It is evident that further search is needed.

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